

**A High-Pressure, High-Temperature Phase Change Induced by Fluorine Chemistry in Mixture Systems with C, H, N, O, F Atoms**

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Chemically reactive systems containing C, H, N, O atoms produce mixtures such as CO, CO<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub>, etc. at high pressure and high temperature. Our earlier calculations predicted that these molecules separate into an N<sub>2</sub>-rich and an N<sub>2</sub>-poor fluid phases. Addition of F atoms, examined in this study, complicates this chemical equilibrium, as they can react with H or C atoms to produce HF or CF<sub>4</sub>. The present chemical equilibrium calculations predict that fluorine occurs mostly as HF in the N<sub>2</sub>-poor phase up to a certain pressure, beyond which it appears mostly as a constituent in CF<sub>4</sub> in the N<sub>2</sub>-rich phase. This shift in fluorine chemistry is often abrupt in thermodynamic sense, enhancing character of the N<sub>2</sub>-fluid phase change. We will discuss relevance of the present prediction to detonation properties of high explosives containing fluorine binders.

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